One-Dimensional Extended States in Partially Disordered Planar Systems

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We obtain analytically a continuum of one-dimensional ballistic extended states in a two-dimensional disordered system, which consists of compactly coupled random and pure square lattices. The extended states give a marginal metallic phase with finite conductivity $\sigma_0 = 2e^2/h$ in a wide energy range, whose boundaries define the mobility edges of a first-order metal-insulator transition. We show current-voltage duality, $H_\parallel/T$ scaling of the conductivity in parallel magnetic field $H_\parallel$ and non-Fermi liquid properties when long-range electron-electron interactions are included.

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Anderson localization and the associated metal-insulator transition (MIT) remain one of the most active fields in condensed matter physics [1]. The one-parameter scaling theory predicts localization of all the states in one or two dimensions for any amount of disorder [2], although even in one-dimension ($1D$) isolated extended states can exist as a consequence of specific short-range disorder correlations [3,4]. In a two-dimensional ($2D$) disordered system delocalization is possible for non-interacting electrons only by breaking the time-reversal symmetry via a magnetic field [5] or the spin-rotation invariance by spin-orbit coupling [6]. Extended states can also appear in continuous $2D$ models with random δ-function potentials of infinitesimal action distance [7]. The presence of extended states in $2D$ random systems is of great interest since metallic phase and MIT has been recently reported in Si-MOS planar structures [8–10] and GaAs-based materials [11], in the absence of magnetic fields.

We analytically show extended wave functions in partially random structure composed of two compactly coupled square lattices, one random and the other periodic. At the same time, according to the scaling theory the rest of the states are localized. Moreover, the extended states have special momentum and form a $1D$ continuum which gives $2e^2/h$ conductivity, in a finite energy range. The boundaries of this range define the mobility edges (ME) of a first-order MIT. These states are perfect (ballistic) and coexist with localized states in their energy range. They correspond to a non-Fermi liquid, in agreement with recent scaling expectations for the presence of a MIT in $2D$ [12]. We show that the system under long-range Coulomb interactions reduces to the marginal Fermi liquid proposed in [13].

We consider two coupled square lattices with the sites of one located above the plaquette centers of the other. One plane is pure and the other is random. The tight-binding Hamiltonian reads

$$H = \sum_{\lambda,i} \epsilon_{\lambda,i} a^\dagger_{\lambda,i} a_{\lambda,i} + \sum_{\lambda,\langle i,j\rangle} t_\lambda (a^\dagger_{\lambda,i} a_{\lambda,j} + \text{H.c.}) + \sum_{\langle 1i,2j\rangle} t (a^\dagger_{1,i} a_{2,j} + \text{H.c.}), \quad (1)$$

where $a_{\lambda,i}$ is the destruction operator for an electron at site i of the $\lambda = 1(2)$ pure (random) plane, t_λ is the nearest-neighbor (NN) hoppings within the λ-th plane and the third term connects each random site to its NN pure sites via the hopping parameter t. We choose $t_1 = t_2 = 1$, setting the energy unit throughout, although our conclusions are also valid if t_2 is random. The sites of the pure plane have energies $\epsilon_{1,i} = 0$ and of the random plane $\epsilon_{2,i}$, randomly distributed between $-W/2$ and $W/2$. For convenience, the length units and the origin of the coordinates are set so that the pure (random) sites count odd (even) numbers.

Obviously, extended wave functions can have zero amplitude on the random sites and finite amplitude on the pure sites, being not influenced by randomness. We can seek for such states in the considered partially disordered system. Indeed, for an $L \times L$ lattice with the described geometry and periodic boundary conditions in all directions, with L even and x_n, y_n the coordinates of the $n \equiv (\lambda, i)$-th site, the states

$$\psi_{1,k_x}(x_n, y_n) = \frac{2}{L} \sin(\frac{y_n \pi}{2}) \exp(i k_x x_n), \quad (2)$$

$$\psi_{2,k_y}(x_n, y_n) = \frac{2}{L} \sin(\frac{x_n \pi}{2}) \exp(i k_y y_n), \quad (3)$$

where $k_x(k_y) = 2j_x(j_y)\pi/L, j_x(j_y) = 1, 2, ..., L/2$, are exact eigenstates of the Hamiltonian H having zero amplitude on the random sites. This can be easily verified

by applying H on $\psi_{1,k_x}(x_n, y_n)$, $\psi_{2,k_y}(x_n, y_n)$ to obtain their eigenenergies

$$E = 2[\cos(2k_x) - 1] \text{ and } E = 2[\cos(2k_y) - 1], \qquad (4)$$

respectively. The transverse momentum of these states is fixed to $k_y(k_x) = \pi/2$ and their longitudinal momentum $k_x(k_y)$ runs in a $1D$ Brillouin zone, forming a $1D$ continuum in the energy range $[-4, 0]$ [14].

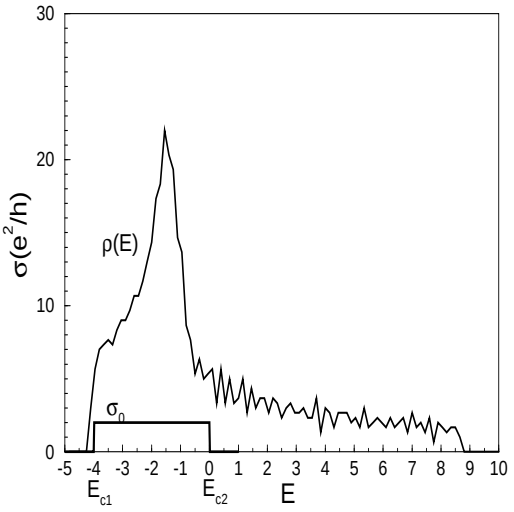

FIG. 1. The density of states $\rho(E)$, in arbitrary units, for a finite $2D$ random sublattice system of linear size $L = 52$ with $t = 1.2$ and $W = 1.5$ by taking averages over 100 random configurations. The scale invariant conductivity σ_0 is also shown.

The perfectly extended states of Eqs. (2) and (3) have momentum along both the $2D$ principal axes and do not violate the scaling theory, since they effectively decouple from the random sites although the two sublattices are compactly coupled. At a given energy E, with $-4 \leq E \leq 0$, they provide propagating channels with $\sigma_0 = 2e^2/h$ conductivity (if spin is included) along the x (or y) direction, independently of the system size L. In Fig. 1 we plot σ_0 and the density of states $\rho(E)$ as a function of E. The rest of the $2D$ states are asymptotically localized, as expected from the scaling theory [2]. The transparent channels give minimum metallic conductivity $\sigma_0 = 2e^2/h$ and one obtains a first-order MIT from σ_0 to 0 at $E_{c1} = -4$ and $E_{c2} = 0$, which can be regarded as mobility edges. For the chosen structure we observe that the lower ME lies near the bottom of the band (see Fig. (1)), so that the Fermi energy can move into the metallic regime even for small electronic doping. For example, this is the case in silicon MOSFETs where the metallic phase is reached at very low electron densities ($\sim 10^{11}\text{cm}^{-2}$) [8–10]. It should be also noted that a minimum metallic conductivity close to e^2/h has been recently suggested, from experimental data in $2D$ hole systems of GaAs heterostructures [15].

The obtained conductivity $\sigma = \sigma_0$ is invariant under scaling so that from the viewpoint of the scaling theory it does not imply a *true* metallic phase for the system, but a critical phase instead, with the corresponding β-function only reaching zero [2]. Moreover, since the extended states coexist with localized states in a wide energy range, having lower dimensionality and measure, we can rename the obtained phase "marginal metallic", following the terminology "marginal Fermi liquid" proposed by Varma *el al* [13].

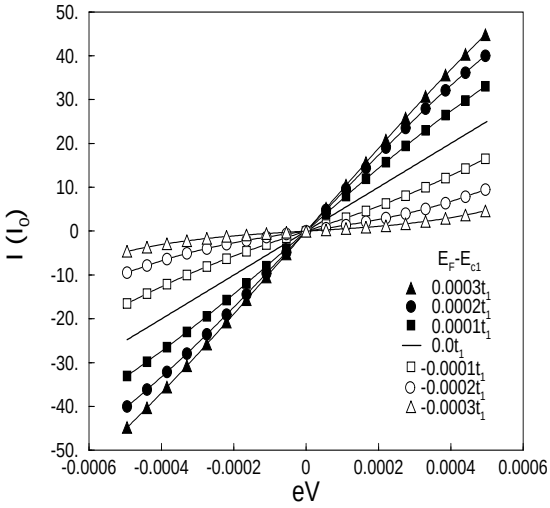

FIG. 2. The current-voltage curves at several Fermi levels around the mobility edge with temperature $k_BT = 1.1 \times 10^{-5} t_1$.

The step-like conductivity $\sigma(E) = \frac{2e^2}{h}\theta(E - E_{c1})$ at E_{c1} gives nonlinearity of the current– voltage $(I - V)$ curves with $I - V$ duality. If the sample is connected to two metallic leads with the same Fermi level E_F, an applied voltage V between the two contacts opens a transmission window of width eV around E_F at zero temperature, due to the electronic occupation in the leads. Nonlinearity occurs if the window boundary passes across the ME when changing the voltage. It becomes smoother at finite temperature T. In order to illustrate this effect we compute the current from the formula

$$I(V) = \frac{I_0}{k_BT}\int_{E_{c1}}^{E_{c_2}} \left(\frac{1}{1 + \exp[(E - E_F - eV/2)/k_BT]} - \frac{1}{1 + \exp[(E - E_F + eV/2)/k_BT]} \right) dE, \qquad (5)$$

where I_0 is a prefactor. In Fig. 2 the calculated $I - V$ curves display nonlinearity if $E_F \neq E_{c1}$. For E_F larger (smaller) than E_{c1} the resistivity increases (decreases)

with $|V|$, giving the symmetric behavior about $E_F = E_{c1}$ known as $I-V$ duality, exchanging the insulating with the metallic phases. Similar kind of duality has been observed in silicon MOSFETs (Fig. 1 of Ref. [10]).

The extended electrons, decoupled from the rest, form a pseudo-Fermi sea embedded in the localized electrons. The pseudo-Fermi surface has only four points corresponding to two Luttinger liquids crossing with each other. This provides a possibility for applying the $1D$ or quasi-$1D$ Luttinger liquid theory to $2D$ systems, as pointed out several years ago [16]. Nevertheless, the system should be regarded as $2D$ non-Fermi liquid owing to its measure, its $1D$-like spectrum, as well as the presence of the background from the localized electrons.

If Coulomb interactions are included the corresponding matrix elements read

$$\langle \mu_1, \mu_2 | V | \mu_3, \mu_4 \rangle = \sum_{\mathbf{n}_1, \mathbf{n}_2} c_1^*(\mathbf{n}_1) c_2^*(\mathbf{n}_2) V(|\mathbf{n}_1 - \mathbf{n}_2|) \; c_3(\mathbf{n}_1) c_4(\mathbf{n}_2), \tag{6}$$

where μ_i is a single-particle state of H and $c_i(\mathbf{n}_j)$ its coefficient at site $\mathbf{n}_j$. We are interested in elements where one of the initial states (μ_3) is extended and the other (μ_4) is localized which describe scattering between extended and localized electrons. The extended states have amplitudes with rapidly changing sign in one direction, while the localized states show no phase coherence having randomly varying amplitudes. Thus, for long-range Coulomb interactions the elements with localized final states μ_1 and μ_2 are almost zero, due to cancellations arising from the positive and negative signs of the extended waves. This leads to an extremely small probability for an extended state to be scattered into a localized state, although the number of localized states is much higher [14]. If a final state (e.g., μ_1) is also extended with the same wave symmetry as the initial state the matrix element is of order ~ 1, since the product $c_1^*(\mathbf{n}_1) c_3(\mathbf{n}_1)$ eliminates the sign of the extended wave coefficients. The above discussion implies that the extended states found can survive in the presence of long-range Coulomb interactions. However, they experience fluctuations from particle-hole excitations of the localized electrons, which can be described by the polarizability

$$\Pi(i\nu_m) \sim 2k_B T \sum_{i,j,\nu_n} G_0(\epsilon_i, i\nu_n) G_0(\epsilon_j, i\nu_n + i\nu_m), \tag{7}$$

where G_0 is the single-particle Green function of the localized states, the sums for i and j are over the relevant localized states for the given interaction, ϵ_i is the energy of state i, and $\nu_n = (2n+1)\pi k_B T$ with n an integer. After summing over the Matsubara frequencies and assuming constant density of the localized states, one has

$$\mathrm{Im}\Pi(\omega) \sim \begin{cases} A_0(\omega/k_B T), \text{ for } |\omega| < k_B T, \\ A_0 \mathrm{sign}\omega, \text{ for } |\omega| > k_B T \end{cases}, \tag{8}$$

where A_0 is a prefactor dependent of density of states. This is the basic hypothesis of the marginal Fermi liquid theory [13]. The key point in this derivation is the momentum independence of the Green function for the localized states. If there are no added impurities in the host sublattice, this manifold is a pure marginal Fermi liquid which can give finite conductivity at zero temperature, distinct from the non-pure marginal Fermi liquid which experiences further impurity scatterings [17].

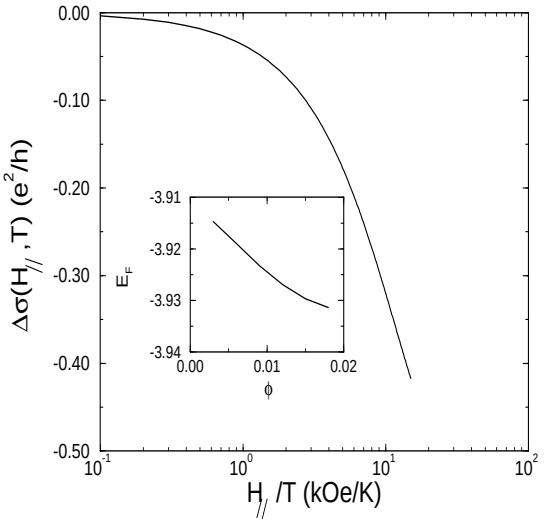

FIG. 3. Main figure: the $H_\parallel/T$ scaling of the conductivity change due to a parallel magnetic field for the system at the transition point. Inset: the Fermi energy E_F vs. ϕ, the flux through a primary inter-plane triangle with the field along the x axis, averaged over 100 random samples with size $L = 30$ ($2 \times 15 \times 15$), and the rest of parameters as in Fig. 1. The units shown are derived for a sample with $a = b = 6$Å, $t_1 = 1$eV. The slope of the inset curve gives $g_1 = -1.1\mu_B$.

An in-plane magnetic field applied to the quasi-$2D$ system in the Coulomb gauge gives in-plane NN hoppings $t_1^{(ij)} = \exp(i\phi \sin\alpha_{ij})$ and $t_2^{(ij)} = \exp(-i\phi \sin\alpha_{ij})$, where α_{ij} is the angle between the hopping bond ij and the field, $\phi = \frac{1}{2} H_\parallel ab$ is the flux through a primary inter-plane triangle, a the planar lattice spacing and b the distance between the planes. The inter-plane NN hoppings are unchanged in this gauge. Thus, the states of Eqs. (2) and (3) survive with eigenenergies $E = 2[\cos(2k_x + 2\phi\sin\alpha_x) - \cos(2\phi\sin\alpha_y)]$ and $E = 2[\cos(2k_y + 2\phi\sin\alpha_y) - \cos(2\phi\sin\alpha_x)]$, respectively, where $\alpha_{x(y)}$ is the angle between the $x(y)$ axis and the field. It can be seen that the shift of E_{c1} (or E_{c2}) is of the order of $H_\parallel^2$ for small fields. At the same time, the whole band including the localized states changes, so that the Fermi level E_F is also shifted if the electron density is kept fixed. In order to obtain the field dependence of E_F we compute the energy spectrum of a finite random

system and the result is shown in the inset of Fig. 3. In general, $\Delta(H_\parallel)$, the energy difference between $E_{c1}(H_\parallel)$ and $E_F(H_\parallel)$, can be expanded as a power series of the field, via $\Delta(H_\parallel) = \Delta(0) + g_1 H_\parallel + ...$ For small fields we can only keep the linear term. On the other hand, the spin degeneracy is removed by $\pm\mu_B H_\parallel$ for up and down spins, with μ_B being the Bohr magneton. For a small bias voltage the conductivity can be expressed in terms of Landauer-Bütticker formula [18] and at the MIT ($\Delta(0) = 0$) one has

$$\sigma(H_\parallel, T) - \sigma(0, T) = \frac{e^2}{h} \sum_{g=\pm 1} \frac{1}{1 + \exp \frac{(g_1 + g\mu_B)H_\parallel}{k_B T}}, \quad (9)$$

which shows $H_\parallel/T$ scaling behavior. In Fig. 3 the $H_\parallel/T$ dependence of conductivity is plotted for one sample, showing good agreement with Fig. 3 of Ref. [19]).

In summary, we have rigorously shown a band of $1D$ ballistic extended states which propagate freely in a $2D$ mixed pure-random system, without magnetic field or spin-orbit coupling. The $1D$ extended continuum is located at the edges of the first Brillouin zone ($k_x = \pi/2$ and any k_y or $k_y = \pi/2$ and any k_x) of the $2D$ square lattice. Moreover, the $1D$ extended states coexist with localized states, in a range of energies whose boundaries define a first-order MIT. We derive $I - V$ duality, $H_\parallel/T$ scaling, and demonstrate non-Fermi or marginal Fermi liquid behavior. These features have not been obtained previously in the presence of disorder and are of profound significance in understanding many experimental findings, especially the $2D$ MIT and the underdoped cuprates. In this Letter we only focus on the general characteristics of a class of partially disordered materials, with at least one sublattice perfect. In Si MOSFETs and GaAs-AlGaAs heterostructures, electrons or holes are confined within several atomic planes and due to lattice mismatch, or atomic diffusion, the planes adjacent to the interface are random, while some planes relatively far from the interface are less random and may support ballistic channels. Another example presents $YBa_2Cu_3O_{6+x}$ where the CuO_2 planes are perfect and the CuO_x planes random due to oxygen vacancies. Although for these materials more realistic models are clearly needed, possibly by including more layers, our results may still shed light on many of their common features.

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